Leticia Gonzalez

List of Publications by Year in Descending Order

346 papers	9,708 citations	50 h-index	81 g-index
374 ext. papers	10,984 ext. citations	5.2 avg, IF	6.72 L-index

#	Paper	IF	Citations
346	Taming Disulfide Bonds with Laser Fields. Nonadiabatic Surface-Hopping Simulations in a Ruthenium Complex.. *Journal of Physical Chemistry Letters*, **2022**, 1894-1900	6.4	2
345	Solvation Effects on the Thermal Helix Inversion of Molecular Motors from QM/MM Calculations. *Chemistry*, **2022**, 4, 185-195	2.1	0
344	Sampling effects in quantum mechanical/molecular mechanics trajectory surface hopping non-adiabatic dynamics.. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2022**, 380, 20200381	3	2
343	HFIP Mediates a Direct C-C Coupling between Michael Acceptors and Eschenmoser's salt. *Angewandte Chemie - International Edition*, **2021**,	16.4	2
342	Simplified State Interaction for Matrix Product State Wave Functions. *Journal of Chemical Theory and Computation*, **2021**,	6.4	1
341	Flexibility Enhances Reactivity: Redox Isomerism and Jahn-Teller Effects in a Bioinspired MnO Cubane Water Oxidation Catalyst. *ACS Catalysis*, **2021**, 11, 13320-13329	13.1	4
340	Jahn-Teller Effects in a Vanadate-Stabilized Manganese-Oxo Cubane Water Oxidation Catalyst. *Chemistry - A European Journal*, **2021**, 27, 17066-17077	4.8	3
339	Strong Ligand Stabilization Based on □Extension in a Series of Ruthenium Terpyridine Water Oxidation Catalysts. *Chemistry - A European Journal*, **2021**, 27, 16871-16878	4.8	2
338	A Force Field for a Manganese-Vanadium Water Oxidation Catalyst: Redox Potentials in Solution as Showcase. *Catalysts*, **2021**, 11, 493	4	1
337	The Role of Triplet States in the Photodissociation of a Platinum Azide Complex by a Density Matrix Renormalization Group Method. *Journal of Physical Chemistry Letters*, **2021**, 12, 4876-4881	6.4	3
336	QM/MM Nonadiabatic Dynamics: the SHARC/COBRAMM Approach. *Journal of Chemical Theory and Computation*, **2021**, 17, 4639-4647	6.4	8
335	Hydrogen-Bond Network Determines the Early Photoisomerization Processes of Cph1 and AnPixJ Phytochromes. *Angewandte Chemie*, **2021**, 133, 18836-18841	3.6	0
334	Photo-Initiated Cobalt-Catalyzed Radical Olefin Hydrogenation. *Chemistry - A European Journal*, **2021**, 27, 16978-16989	4.8	1
333	Hydrogen-Bond Network Determines the Early Photoisomerization Processes of Cph1 and AnPixJ Phytochromes. *Angewandte Chemie - International Edition*, **2021**, 60, 18688-18693	16.4	2
332	Meyer-Schuster-type rearrangement for the synthesis of □selanyl-□unsaturated thioesters. *Chemical Communications*, **2021**, 57, 117-120	5.8	3
331	Ultrafast photochemistry of a molybdenum carbonyl-nitrosyl complex with a triazacyclononane coligand. *Physical Chemistry Chemical Physics*, **2021**, 23, 24187-24199	3.6	0
330	The importance of finite temperature and vibrational sampling in the absorption spectrum of a nitro-functionalized Ru(ii) water oxidation catalyst. *Physical Chemistry Chemical Physics*, **2021**, 23, 17724-17733	3.6	0

329	Ultrafast and long-time excited state kinetics of an NIR-emissive vanadium(iii) complex II. Elucidating triplet-to-singlet excited-state dynamics. *Chemical Science*, **2021**, 12, 10791-10801	9.4	11
328	Excited-State Dynamics of [Ru(bpy)(bpy)] to Form Long-Lived Localized Triplet States. *Inorganic Chemistry*, **2021**, 60, 1672-1682	5.1	8
327	Excited-State Properties and Relaxation Pathways of Selenium-Substituted Guanine Nucleobase in Aqueous Solution and DNA Duplex. *Journal of Physical Chemistry B*, **2021**, 125, 1778-1789	3.4	5
326	Validating fewest-switches surface hopping in the presence of laser fields. *Journal of Chemical Physics*, **2021**, 154, 144102	3.9	4
325	The Quest to Simulate Excited-State Dynamics of Transition Metal Complexes. *Jacs Au*, **2021**, 1, 1116-1140		11
324	A Ruthenium(II) Water Oxidation Catalyst Containing a pH-Responsive Ligand Framework. *Inorganic Chemistry*, **2021**, 60, 13299-13308	5.1	1
323	A Density Matrix Renormalization Group Study of the Low-Lying Excited States of a Molybdenum Carbonyl-Nitrosyl Complex. *ChemPhysChem*, **2021**, 22, 2371-2377	3.2	
322	Spectral Signatures of Oxidation States in a Manganese-Oxo Cubane Water Oxidation Catalyst. *Chemistry - A European Journal*, **2021**, 27, 17078-17086	4.8	2
321	Surface Hopping Dynamics on Vibronic Coupling Models. *Accounts of Chemical Research*, **2021**, 54, 3760-3771	24.3	8
320	On the population of triplet states of 2-seleno-thymine. *Physical Chemistry Chemical Physics*, **2021**, 23, 5447-5454	3.6	1
319	Activation by oxidation and ligand exchange in a molecular manganese vanadium oxide water oxidation catalyst. *Chemical Science*, **2021**, 12, 12918-12927	9.4	5
318	Implementation of Coherent Switching with Decay of Mixing into the SHARC Program. *Journal of Chemical Theory and Computation*, **2020**, 16, 3464-3475	6.4	9
317	Spiropyran Meets Guanine Quadruplexes: Isomerization Mechanism and DNA Binding Modes of Quinolizidine-Substituted Spiropyran Probes. *Chemistry - A European Journal*, **2020**, 26, 13039-13045	4.8	6
316	Orbital-free photophysical descriptors to predict directional excitations in metal-based photosensitizers. *Chemical Science*, **2020**, 11, 7685-7693	9.4	6
315	Unveiling the reaction mechanism of novel copper N-alkylated tetra-azacyclophanes with outstanding superoxide dismutase activity. *Chemical Communications*, **2020**, 56, 7511-7514	5.8	4
314	Competing ultrafast photoinduced electron transfer and intersystem crossing of [Re(CO)(Dmp)(His124)(Trp122)] in azurin: a nonadiabatic dynamics study. *Theoretical Chemistry Accounts*, **2020**, 139, 65	1.9	11
313	Electrochemical and Photophysical Properties of Ruthenium(II) Complexes Equipped with Sulfurated Bipyridine Ligands. *Inorganic Chemistry*, **2020**, 59, 4972-4984	5.1	10
312	Biological evaluation of novel thiomaltol-based organometallic complexes as topoisomerase II inhibitors. *Journal of Biological Inorganic Chemistry*, **2020**, 25, 451-465	3.7	8

311	CASPT2 Potential Energy Curves for NO Dissociation in a Ruthenium Nitrosyl Complex. *Molecules*, **2020**, 25,	4.8	6
310	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. *Journal of Chemical Physics*, **2020**, 152, 134110	3.9	22
309	Early Relaxation Dynamics in the Photoswitchable Complex trans-[RuCl(NO)(py)]. *Chemistry - A European Journal*, **2020**, 26, 11522-11528	4.8	12
308	A Vanadium(III) Complex with Blue and NIR-II Spin-Flip Luminescence in Solution. *Journal of the American Chemical Society*, **2020**, 142, 7947-7955	16.4	41
307	Equation-of-Motion Coupled-Cluster Models **2020**, 77-108		2
306	Multi-Reference Configuration Interaction **2020**, 277-297		1
305	Molekulare Photochemie: Moderne Entwicklungen in der theoretischen Chemie. *Angewandte Chemie*, **2020**, 132, 16976-16992	3.6	1
304	Revealing Ultrafast Population Transfer between Nearly Degenerate Electronic States. *Journal of Physical Chemistry Letters*, **2020**, 11, 1443-1449	6.4	3
303	Enhanced Rigidity Changes Ultraviolet Absorption: Effect of a Merocyanine Binder on G-Quadruplex Photophysics. *Journal of Physical Chemistry Letters*, **2020**, 11, 10212-10218	6.4	8
302	Funktionalisierung von Ketonen durch metallfreie elektrophile Aktivierung. *Angewandte Chemie*, **2020**, 132, 21121-21125	3.6	2
301	Path-Integral Approaches to Non-Adiabatic Dynamics **2020**, 629-653		3
300	Multi-Configurational Density Functional Theory: Progress and Challenges **2020**, 47-75		1
299	The effect of N-heterocyclic carbene units on the absorption spectra of Fe(II) complexes: a challenge for theory. *Physical Chemistry Chemical Physics*, **2020**, 22, 27605-27616	3.6	5
298	Bohmian Approaches to Non-Adiabatic Molecular Dynamics **2020**, 563-594		0
297	Time-Dependent Density Functional Theory **2020**, 13-46		6
296	Exact Quantum Dynamics (Wave Packets) in Reduced Dimensionality **2020**, 355-381		4
295	Full and Ab Initio Multiple Spawning **2020**, 435-467		3
294	Surface Hopping Molecular Dynamics **2020**, 499-530		4

293	Exact Factorization of the Electron□Nuclear Wave Function: Theory and Applications **2020**, 531-562		6
292	Excimer Intermediates en Route to Long-Lived Charge-Transfer States in Single-Stranded Adenine DNA as Revealed by Nonadiabatic Dynamics. *Journal of Physical Chemistry Letters*, **2020**, 11, 7483-7488	6.4	12
291	Intersystem Crossing and Triplet Dynamics in an Iron(II) N-Heterocyclic Carbene Photosensitizer. *Inorganic Chemistry*, **2020**, 59, 14666-14678	5.1	13
290	Site-Specific Photo-oxidation of the Isolated Adenosine-5'-triphosphate Dianion Determined by Photoelectron Imaging. *Journal of Physical Chemistry Letters*, **2020**, 11, 8195-8201	6.4	3
289	□Functionalisation of Ketones Through Metal-Free Electrophilic Activation. *Angewandte Chemie - International Edition*, **2020**, 59, 20935-20939	16.4	17
288	Motivation and Basic Concepts **2020**, 1-12		
287	Multi-Configuration Time-Dependent Hartree Methods: From Quantum to Semiclassical and Quantum-Classical **2020**, 383-411		3
286	Gaussian Wave Packets and the DD-vMCG Approach **2020**, 413-433		1
285	Semiclassical Molecular Dynamics for Spectroscopic Calculations **2020**, 595-628		11
284	Multi-Configurational Reference Perturbation Theory with a CASSCF Reference Function **2020**, 299-353		3
283	The Algebraic-Diagrammatic Construction Scheme for the Polarization Propagator **2020**, 109-131		2
282	Foundation of Multi-Configurational Quantum Chemistry **2020**, 133-203		3
281	The Density Matrix Renormalization Group for Strong Correlation in Ground and Excited States **2020**, 205-245		7
280	Excited-State Calculations with Quantum Monte Carlo **2020**, 247-275		6
279	Molecular Photochemistry: Recent Developments in Theory. *Angewandte Chemie - International Edition*, **2020**, 59, 16832-16846	16.4	55
278	Directional and regioselective hole injection of spiropyran photoswitches intercalated into A/T-duplex DNA. *Physical Chemistry Chemical Physics*, **2019**, 21, 17971-17977	3.6	6
277	From Surface Hopping to Quantum Dynamics and Back. Finding Essential Electronic and Nuclear Degrees of Freedom and Optimal Surface Hopping Parameters. *Journal of Physical Chemistry A*, **2019**, 123, 8321-8332	2.8	13
276	OpenMolcas: From Source Code to Insight. *Journal of Chemical Theory and Computation*, **2019**, 15, 5925-5964	5.5	310

275	Solvent reorganization triggers photo-induced solvated electron generation in phenol. *Physical Chemistry Chemical Physics*, **2019**, 21, 14261-14269	3.6	6
274	A redox-neutral synthesis of ketones by coupling of alkenes and amides. *Nature Communications*, **2019**, 10, 2327	17.4	14
273	Nonadiabatic Dynamics Simulation Predict Intersystem Crossing in Nitroaromatic Molecules on a Picosecond Time Scale. *ChemPhotoChem*, **2019**, 3, 833-845	3.3	4
272	The Influence of the Electronic Structure Method on Intersystem Crossing Dynamics. The Case of Thioformaldehyde. *Journal of Chemical Theory and Computation*, **2019**, 15, 3470-3480	6.4	19
271	Curious Case of 2-Selenouracil: Efficient Population of Triplet States and Yet Photostable. *Journal of Chemical Theory and Computation*, **2019**, 15, 3730-3742	6.4	9
270	The 3s Rydberg state as a doorway state in the ultrafast dynamics of 1,1-difluoroethylene. *Physical Chemistry Chemical Physics*, **2019**, 21, 4871-4878	3.6	1
269	A XMS-CASPT2 non-adiabatic dynamics study on pyrrole. *Computational and Theoretical Chemistry*, **2019**, 1155, 38-46	2	14
268	Machine learning enables long time scale molecular photodynamics simulations. *Chemical Science*, **2019**, 10, 8100-8107	9.4	96
267	Strong Influence of Decoherence Corrections and Momentum Rescaling in Surface Hopping Dynamics of Transition Metal Complexes. *Journal of Chemical Theory and Computation*, **2019**, 15, 5031-5045	6.4	34
266	Reaction mechanism of nucleoside 2'-deoxyribosyltransferases: free-energy landscape supports an oxocarbenium ion as the reaction intermediate. *Organic and Biomolecular Chemistry*, **2019**, 17, 7891-7899	3.9	6
265	Unified Approach to the Chemoselective □-Functionalization of Amides with Heteroatom Nucleophiles. *Journal of the American Chemical Society*, **2019**, 141, 18437-18443	16.4	34
264	Molecular light switch effect in Ru(II) complexes intercalated in DNA: a theoretical study **2019**, 778-779		
263	The Reactivity and Stability of Polyoxometalate Water Oxidation Electrocatalysts. *Molecules*, **2019**, 25,	4.8	27
262	DNA-binding mechanism of spiropyran photoswitches: the role of electrostatics. *Physical Chemistry Chemical Physics*, **2019**, 21, 8614-8618	3.6	3
261	Unconventional two-step spin relaxation dynamics of [Re(CO)(im)(phen)] in aqueous solution. *Chemical Science*, **2019**, 10, 10405-10411	9.4	23
260	Identification of important normal modes in nonadiabatic dynamics simulations by coherence, correlation, and frequency analyses. *Journal of Chemical Physics*, **2019**, 151, 244115	3.9	9
259	Finite-temperature Wigner phase-space sampling and temperature effects on the excited-state dynamics of 2-nitronaphthalene. *Physical Chemistry Chemical Physics*, **2019**, 21, 13906-13915	3.6	18
258	Exploring density functional subspaces with genetic algorithms. *Monatshefte Fü Chemie*, **2019**, 150, 173-182	1.4	6

257	The Role of Electronic Triplet States and High-Lying Singlet States in the Deactivation Mechanism of the Parent BODIPY: An ADC(2) and CASPT2 Study. *ChemPhotoChem*, **2019**, 3, 727-738	3.3	15
256	Highly efficient surface hopping dynamics using a linear vibronic coupling model. *Physical Chemistry Chemical Physics*, **2018**, 21, 57-69	3.6	55
255	Solvent Effects on Electronically Excited States: QM/Continuum Versus QM/Explicit Models. *Journal of Physical Chemistry B*, **2018**, 122, 2975-2984	3.4	16
254	Computational Photophysics in the Presence of an Environment. *Annual Review of Physical Chemistry*, **2018**, 69, 473-497	15.7	36
253	Vibrational Sampling and Solvent Effects on the Electronic Structure of the Absorption Spectrum of 2-Nitronaphthalene. *Journal of Chemical Theory and Computation*, **2018**, 14, 3205-3217	6.4	15
252	Unusual mechanisms in Claisen rearrangements: an ionic fragmentation leading to a -selective rearrangement. *Chemical Science*, **2018**, 9, 4124-4131	9.4	20
251	Quantitative wave function analysis for excited states of transition metal complexes. *Coordination Chemistry Reviews*, **2018**, 361, 74-97	23.2	81
250	Mechanism of Ultrafast Intersystem Crossing in 2-Nitronaphthalene. *Chemistry - A European Journal* , **2018**, 24, 5379-5387	4.8	35
249	Exciton Localization on Ru-Based Photosensitizers Induced by Binding to Lipid Membranes. *Journal of Physical Chemistry Letters*, **2018**, 9, 683-688	6.4	10
248	Hydrative Aminoxylation of Ynamides: One Reaction, Two Mechanisms. *Chemistry - A European Journal*, **2018**, 24, 2515-2519	4.8	14
247	Interstate vibronic coupling constants between electronic excited states for complex molecules. *Journal of Chemical Physics*, **2018**, 148, 124119	3.9	21
246	Visible light-induced cis/trans isomerization of dicarbonyl Fe(II) PNP pincer complexes. *Polyhedron*, **2018**, 143, 94-98	2.7	1
245	Shedding Light on the Nature of Photoinduced States Formed in a Hydrogen-Generating Supramolecular RuPt Photocatalyst by Ultrafast Spectroscopy. *Journal of Physical Chemistry A*, **2018** , 122, 6396-6406	2.8	6
244	Nonadiabatic dynamics: The SHARC approach. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1370	7.9	158
243	Intersystem Crossing as a Key Component of the Nonadiabatic Relaxation Dynamics of Bithiophene and Terthiophene. *Journal of Chemical Theory and Computation*, **2018**, 14, 4530-4540	6.4	10
242	Effect of DNA Environment on Electronically Excited States of Methylene Blue Evaluated by a Three-Layered QM/QM/MM ONIOM Scheme. *Journal of Chemical Theory and Computation*, **2018**, 14, 4298-4308	6.4	12
241	Stepwise photosensitized thymine dimerization mediated by an exciton intermediate. *Monatshefte F□ Chemie*, **2018**, 149, 1-9	1.4	13
240	A Valence-Delocalised Osmium Dimer capable of Dinitrogen Photocleavage: Ab Initio Insights into Its Electronic Structure. *Chemistry - A European Journal*, **2018**, 24, 5112-5123	4.8	9

239	Assessing Configurational Sampling in the Quantum Mechanics/Molecular Mechanics Calculation of Temoporfin Absorption Spectrum and Triplet Density of States. *Molecules*, **2018**, 23,	4.8	7
238	Novel Molecular-Dynamics-Based Protocols for Phase Space Sampling in Complex Systems. *Frontiers in Chemistry*, **2018**, 6, 495	5	21
237	Wavelength-optimized Two-Photon Polymerization Using Initiators Based on Multipolar Aminostyryl-1,3,5-triazines. *Scientific Reports*, **2018**, 8, 17273	4.9	23
236	Surface Hopping within an Exciton Picture. An Electrostatic Embedding Scheme. *Journal of Chemical Theory and Computation*, **2018**, 14, 6139-6148	6.4	22
235	Simulated and Experimental Time-Resolved Photoelectron Spectra of the Intersystem Crossing Dynamics in 2-Thiouracil. *Molecules*, **2018**, 23,	4.8	19
234	Cover Image, Volume 8, Issue 6. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1400	7.9	7
233	Enhancing the Stability of Photogenerated Benzophenone Triplet Radical Pairs through Supramolecular Assembly. *Journal of the American Chemical Society*, **2018**, 140, 13064-13070	16.4	11
232	Hydrogen Bonding Regulates the Rigidity of Liposome-Encapsulated Chlorin Photosensitizers. *ChemistryOpen*, **2018**, 7, 475-483	2.3	9
231	An Asymmetric Redox Arylation: Chirality Transfer from Sulfur to Carbon through a Sulfonium [3,3]-Sigmatropic Rearrangement. *Angewandte Chemie - International Edition*, **2017**, 56, 2212-2215	16.4	88
230	Impact of Lipid Environment on Photodamage Activation of Methylene Blue. *ChemPhotoChem*, **2017**, 1, 178-182	3.3	13
229	Asymmetrische Redoxarylierung: Chiralitätstransfer von Schwefel zu Kohlenstoff durch sigmatrope Sulfonium-[3,3]-Umlagerung. *Angewandte Chemie*, **2017**, 129, 2248-2252	3.6	32
228	Ab initio molecular dynamics relaxation and intersystem crossing mechanisms of 5-azacytosine. *Physical Chemistry Chemical Physics*, **2017**, 19, 5888-5894	3.6	24
227	Sequential Proton-Coupled Electron Transfer Mediates Excited-State Deactivation of a Eumelanin Building Block. *Journal of Physical Chemistry Letters*, **2017**, 8, 1004-1008	6.4	23
226	Discrimination of 1,1-difluoroethylene nuclear spin isomers in the presence of non-adiabatic coupling terms. *Chemical Physics Letters*, **2017**, 683, 205-210	2.5	2
225	Direct Determination of Metal Complexes' Interaction with DNA by Atomic Telemetry and Multiscale Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2017**, 8, 805-811	6.4	16
224	Direct Regioselective Synthesis of Tetrazolium Salts by Activation of Secondary Amides under Mild Conditions. *Organic Letters*, **2017**, 19, 2662-2665	6.2	35
223	Solvatochromic Effects on the Absorption Spectrum of 2-Thiocytosine. *Journal of Physical Chemistry B*, **2017**, 121, 5187-5196	3.4	19
222	2-Thiouracil intersystem crossing photodynamics studied by wavelength-dependent photoelectron and transient absorption spectroscopies. *Physical Chemistry Chemical Physics*, **2017**, 19, 19756-19766	3.6	43

221	Electronic delocalization, charge transfer and hypochromism in the UV absorption spectrum of polyadenine unravelled by multiscale computations and quantitative wavefunction analysis. *Chemical Science*, **2017**, 8, 5682-5691	9.4	61
220	Insights into the deactivation of 5-bromouracil after ultraviolet excitation. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2017**, 375,	3	7
219	Excited-states of a rhenium carbonyl diimine complex: solvation models, spin-orbit coupling, and vibrational sampling effects. *Physical Chemistry Chemical Physics*, **2017**, 19, 27240-27250	3.6	36
218	Detailed Wave Function Analysis for Multireference Methods: Implementation in the Molcas Program Package and Applications to Tetracene. *Journal of Chemical Theory and Computation*, **2017** , 13, 5343-5353	6.4	32
217	Publisher's Note: Molecular oxygen observed by direct photoproduction from carbon dioxide [Phys. Rev. A 95, 011404(R) (2017)]. *Physical Review A*, **2017**, 95,	2.6	2
216	Laser-Induced Oxygen Formation from Carbon Dioxide. *Journal of Physics: Conference Series*, **2017**, 875, 032024	0.3	
215	Ab initio molecular dynamics of thiophene: the interplay of internal conversion and intersystem crossing. *Physical Chemistry Chemical Physics*, **2017**, 19, 25662-25670	3.6	25
214	Molecular oxygen observed by direct photoproduction from carbon dioxide. *Physical Review A*, **2017**, 95,	2.6	7
213	Intramolecular hydrogen bonding in conformationally semi-rigid β-acylmethane derivatives: a theoretical NMR study. *Organic and Biomolecular Chemistry*, **2017**, 15, 7572-7579	3.9	1
212	Trajectory Surface-Hopping Dynamics Including Intersystem Crossing in [Ru(bpy)]. *Journal of Physical Chemistry Letters*, **2017**, 8, 3840-3845	6.4	81
211	Assessing Excited State Energy Gaps with Time-Dependent Density Functional Theory on Ru(II) Complexes. *Journal of Chemical Theory and Computation*, **2017**, 13, 4123-4145	6.4	33
210	Surface hopping dynamics including intersystem crossing using the algebraic diagrammatic construction method. *Journal of Chemical Physics*, **2017**, 147, 184109	3.9	23
209	Linkage Photoisomerization Mechanism in a Photochromic Ruthenium Nitrosyl Complex: New Insights from an MS-CASPT2 Study. *Journal of Chemical Theory and Computation*, **2017**, 13, 6120-6130	6.4	23
208	Mechanistic Pathways in Amide Activation: Flexible Synthesis of Oxazoles and Imidazoles. *Organic Letters*, **2017**, 19, 3815-3818	6.2	29
207	The IPEA dilemma in CASPT2. *Chemical Science*, **2017**, 8, 1482-1499	9.4	134
206	The DNA nucleobase thymine in motion—intersystem crossing simulated with surface hopping. *Chemical Physics*, **2017**, 482, 9-15	2.3	27
205	Challenges in Simulating Light-Induced Processes in DNA. *Molecules*, **2017**, 22, 49	4.8	13
204	Metal-Free meta-Selective Alkyne Oxyarylation with Pyridine N-Oxides: Rapid Assembly of Metyrapone Analogues. *Angewandte Chemie - International Edition*, **2016**, 55, 15424-15428	16.4	30

203	Metal-free intermolecular formal cycloadditions enable an orthogonal access to nitrogen heterocycles. *Nature Communications*, **2016**, 7, 10914	17.4	72
202	The origin of efficient triplet state population in sulfur-substituted nucleobases. *Nature Communications*, **2016**, 7, 13077	17.4	110
201	Revealing Deactivation Pathways Hidden in Time-Resolved Photoelectron Spectra. *Scientific Reports*, **2016**, 6, 35522	4.9	21
200	Ruthenium Carbonyl Complexes with Azole Heterocycles Synthesis, X-ray Diffraction Structures, DFT Calculations, Solution Behavior, and Antiproliferative Activity. *European Journal of Inorganic Chemistry*, **2016**, 2016, 1566-1576	2.3	6
199	Peripheral ligands as electron storage reservoirs and their role in enhancement of photocatalytic hydrogen generation. *Chemical Communications*, **2016**, 52, 9371-4	5.8	18
198	Divergent ynamide reactivity in the presence of azides - an experimental and computational study. *Chemical Science*, **2016**, 7, 6032-6040	9.4	28
197	Chemo- and Stereoselective Transition-Metal-Free Amination of Amides with Azides. *Journal of the American Chemical Society*, **2016**, 138, 8348-51	16.4	87
196	Controlling the Excited-State Dynamics of Nuclear Spin Isomers Using the Dynamic Stark Effect. *Journal of Physical Chemistry A*, **2016**, 120, 4907-14	2.8	3
195	Efficient and Flexible Computation of Many-Electron Wave Function Overlaps. *Journal of Chemical Theory and Computation*, **2016**, 12, 1207-19	6.4	100
194	Benzophenone Ultrafast Triplet Population: Revisiting the Kinetic Model by Surface-Hopping Dynamics. *Journal of Physical Chemistry Letters*, **2016**, 7, 622-6	6.4	71
193	Communication: GAIMS--Generalized Ab Initio Multiple Spawning for both internal conversion and intersystem crossing processes. *Journal of Chemical Physics*, **2016**, 144, 101102	3.9	74
192	Communication: Unambiguous comparison of many-electron wavefunctions through their overlaps. *Journal of Chemical Physics*, **2016**, 145, 021103	3.9	17
191	Photoelectron spectra of 2-thiouracil, 4-thiouracil, and 2,4-dithiouracil. *Journal of Chemical Physics*, **2016**, 144, 074303	3.9	37
190	Internal conversion and intersystem crossing pathways in UV excited, isolated uracils and their implications in prebiotic chemistry. *Physical Chemistry Chemical Physics*, **2016**, 18, 20168-76	3.6	50
189	Intersystem Crossing Pathways in the Noncanonical Nucleobase 2-Thiouracil: A Time-Dependent Picture. *Journal of Physical Chemistry Letters*, **2016**, 7, 1978-83	6.4	97
188	Cyclobutane Thymine Photodimerization Mechanism Revealed by Nonadiabatic Molecular Dynamics. *Journal of the American Chemical Society*, **2016**, 138, 15911-15916	16.4	48
187	Orbital entanglement and CASSCF analysis of the Ru-NO bond in a Ruthenium nitrosyl complex. *Physical Chemistry Chemical Physics*, **2015**, 17, 14383-92	3.6	49
186	Quenching of Charge Transfer in Nitrobenzene Induced by Vibrational Motion. *Journal of Physical Chemistry Letters*, **2015**, 6, 3006-11	6.4	20

185	Separating nuclear spin isomers using a pump□ump laser scheme. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	3
184	Electronic and structural elements that regulate the excited-state dynamics in purine nucleobase derivatives. *Journal of the American Chemical Society*, **2015**, 137, 4368-81	16.4	58
183	Using computational chemistry to design Ru photosensitizers with directional charge transfer. *Coordination Chemistry Reviews*, **2015**, 304-305, 146-165	23.2	48
182	A Static Picture of the Relaxation and Intersystem Crossing Mechanisms of Photoexcited 2-Thiouracil. *Journal of Physical Chemistry A*, **2015**, 119, 9524-33	2.8	55
181	A general method to describe intersystem crossing dynamics in trajectory surface hopping. *International Journal of Quantum Chemistry*, **2015**, 115, 1215-1231	2.1	178
180	Steigerung der Interkombinationseffizienz in Phenothiazinfarbstoffen durch Einlagerung in DNA. *Angewandte Chemie*, **2015**, 127, 4450-4453	3.6	8
179	Origin of the Regioselectivity in the Gas-Phase Aniline+CH3 (+) Electrophilic Aromatic Substitution. *ChemPhysChem*, **2015**, 16, 2366-74	3.2	
178	Time-resolved insight into the photosensitized generation of singlet oxygen in endoperoxides. *Journal of Chemical Theory and Computation*, **2015**, 11, 406-14	6.4	20
177	Enhancing intersystem crossing in phenotiazinium dyes by intercalation into DNA. *Angewandte Chemie - International Edition*, **2015**, 54, 4375-8	16.4	45
176	Unravelling the quenching mechanisms of a luminescent Ru(II) probe for Cu(II). *Chemistry - an Asian Journal*, **2015**, 10, 622-9	4.5	7
175	Excitation of nucleobases from a computational perspective II: dynamics. *Topics in Current Chemistry*, **2015**, 355, 99-153		37
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